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Techno-economic analysis of biobased chemicals production via integrated catalytic processing

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We calculate the internal rate of return (IRR) for each scenario as functions of the costs of feedstock, hydrogen, and catalyst, and projected revenues for the facility. The assumed feedstock cost is $83/MT for mixed wood. The assumed hydrogen cost is $3/kg. Catalyst costs are based on December 2010 prices and projected revenues are based on August 2010 petrochemical prices.

The analysis indicates that a facility employing FCC of WPO or APPO without hydrotreating is unable to generate a positive IRR. Employment of two-stage hydrotreating significantly increases the facility IRR, although IRRs in excess of 10% are only attained when higher pyrolysis oil yields (70 wt%) are assumed.

Keywords
fast pyrolysis, integrated catalytic processing, biobased chemicals, pyrolysis oil, Bioeconomy Institute, Mechanical Engineering

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Technoeconomic Analysis of Biobased Chemicals Production via Integrated Catalytic Processing

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Introduction

Concerns about the environment, dependency on foreign petroleum production, and persistent high petroleum prices have spurred research into technologies for the production of transportation fuels from non-food biomass. This research has focused on carbohydrate feedstocks to produce ethanol, which can legally replace 10-15% of the gasoline used in internal combustion engines in the U.S.;[1] higher blends may only be used in modified vehicles as they can damage the engine and fuel system of conventional vehicles. Recent research has focused on drop-in biofuels, so-called for their ability to fully replace petroleum-based transportation fuels in the existing transportation fuel infrastructure. While drop-in biofuels can be produced via a number of pathways and from a variety of feedstocks, fast pyrolysis has attracted attention due to prospects for distributed deployment of biomass processing systems,[(2)] its attractive economics,[(3)] and the ability to return soil nutrients as part of the fuel production cycle.[(4)] Fast pyrolysis results in three products: solid (char also known as biochar), gas (syngas also known as non-condensable gas), and liquid (pyrolysis oil also known as bio-oil). Pyrolysis oil is produced from condensable vapors and liquid aerosols released during pyrolysis. Commercial applications at present include the production of bioasphalt (Avello Bioenergy) and transportation fuels (KiOR). While char currently has little market value and syngas is used to generate facility process heat, pyrolysis oil can be refined into biobased hydrocarbons such as gasoline and diesel at a cost range of $1.74-$3.09/gallon.[(5, 6)] The profitability of a fast pyrolysis facility depends on its ability to utilize pyrolysis oil as a feedstock for high-value products, such as drop-in biofuels.[(7)]

Recent research has found that pyrolysis oil can serve as a feedstock for many of the products of the petrochemical industry, such as benzene, toluene, and xylene (BTX).[(8-10)] The petrochemical industry was responsible for only 2.5% of U.S. petroleum consumption[(11)] and 0.05% of U.S.

greenhouse gas emissions in 2008.[12] Nevertheless, prices of many petrochemical products are higher than that of gasoline,[13, 14] making production of biobased chemicals an attractive use of pyrolysis oil.

Pyrolysis oil has several applications including power generation[15-17] and production of fuels,[5-7, 18-21] hydrogen,[22-24] commodity chemicals,[9, 10, 25-29] and polymers.[6, 30] Co-product char has received international attention [31-33] due to its CO_2 sequestration properties.[7, 34-36] Char can also be used to generate power either within the pyrolysis facility[6] or in a dedicated power plant.[17] The gaseous product, syngas, is most commonly used to generate process heat within the pyrolysis facility as its high CO content makes it unsuitable for many commercial applications.

Production of drop-in biofuels from pyrolysis oil is attractive due to its use of inexpensive and plentiful lignocellulosic biomass as feedstock[6, 26] and the low cost of the resulting fuels relative to other advanced biofuel pathways.[37] Pyrolysis oil also has disadvantages that have impeded its substitution for petroleum. Raw pyrolysis oil is viscous, corrosive, unstable, and highly oxygenated,[20, 38-40] making it difficult to transport, store, and refine.[41, 42]

Furthermore, pyrolysis oil must be substantially or completely deoxygenated before it can substitute for petroleum. This is ideally accomplished in a single unit operation, simplifying the process and reducing both capital and operating costs. A prominent example is fluid catalytic cracking (FCC), which uses a zeolite catalyst to decarboxylate and decarbonate oxygenated molecules without the addition of hydrogen to yield hydrocarbons.[19] However, the wide range of chemical moieties including both monomeric and oligomeric species results in relatively low product yields of specific product molecules. Upgrading pyrolysis oil in multiple unit operations improves yields albeit at additional processing cost.[10] The addition of hydrogen

(hydroprocessing, which encompasses both hydrotreating and hydrocracking) is usually involved in at least one step. Often the first step is hydrotreating, which uses hydrogen at relatively modest temperatures in the presence of a catalyst to remove heteronuclear atoms from the pyrolysis oil molecules, especially oxygen but also nitrogen, sulfur, and chlorine.[20] The removal of carboxylic functionality reduces the corrosiveness of the pyrolysis oil as well as the viscosity.[5]

Pyrolysis oil includes oligomers derived from both carbohydrate and lignin, some of which remains even after deoxygenation of the oil. Generally, these "heavy ends" must be depolymerized to smaller molecules suitable as transportation fuel or commodity chemicals. This depolymerization step can be attained via either hydrocracking or FCC. Hydrocracking, like hydrotreating, reacts pyrolysis oil with hydrogen in the presence of a catalyst but under more severe reaction conditions with the purpose of breaking carbon bonds in long-chained or cyclic compounds to produce relatively short-chain hydrocarbons suitable for fuels.[43]

Hydrotreating involves significant hydrogen consumption, in the range of 0.05-0.09 kg/kg pyrolysis oil just to prepare the raw pyrolysis oil for conventional refining.[44] Additional hydrocracking is necessary to produce the final transportation fuel products from the pyrolysis oil. This hydrogen consumption can represent a substantial contribution to operating expenses, particularly when hydrogen prices are high. FCC incurs lower operating costs but suffers from high coke formation on the catalyst, requiring frequent catalyst regeneration and limiting the catalyst life.[45] Additionally, some studies have reported potential hydrocarbon yields from FCC to be lower than those from hydroprocessing.[43, 46]

Vispute et al.[10] have recently proposed to combine hydrotreating and FCC of pyrolysis oil in a process known as Integrated Catalytic Processing (ICP). In experiments with pyrolysis oil

produced from mixed woods, it was found that hydrotreating whole pyrolysis oil (WPO) or the aqueous phase of pyrolysis oil (APPO) over a Ru/C catalyst at 398 K and 100 bar (WPO) or 52 bar (APPO) pressure prior to FCC reduced coke production by up to 46% and increased yields of aromatic hydrocarbons (benzene, toluene, xylene, and ethyl benzene) and olefins (ethylene, propylene, and butylene) up to 36% compared to direct FCC processing. Two-stage hydrotreating involved hydrotreating the APPO over a Ru/C catalyst at 398 K and 52 bar pressure followed by a second, higher temperature stage of hydrotreating with a Pt/C catalyst at 523 K and 100 bar pressure prior to FCC. This two-stage hydrotreating process further reduced coke yields and increased aromatic hydrocarbon and olefin yields. In all scenarios FCC occurred over an HZSM-5 catalyst at 873K and atmospheric pressure. In comparing the market price of the resulting commodity chemicals to the estimated cost of the biomass feedstock cost, Vispute et al.[10] concluded that one or more hydrotreating stages prior to FCC were economically attractive by calculating the "economic potential" of each scenario. This was calculated by subtracting the cost of biomass and hydrogen from the selling price of the commodity chemical products, with no accounting of any capital or other operating costs.[10] Pyrolysis oil yields were assumed to be 70 wt% for each scenario. Assuming a $2/kg price for hydrogen, Vispute et al. calculated the annual economic potential (defined as the product selling price minus feedstock and hydrogen costs) of Scenario 1 to be ~$18 million, of Scenario 2 to be a ~$19 million, of Scenario 3 to be ~$20 million, of Scenario 4 to be ~$50 million, and of Scenario 5 to be ~$70 million. These are relatively attractive economic potentials, but the analysis does not account for capital costs or operating costs other than feedstock.

The objective of this paper is to provide a detailed economic analysis of the potential of ICP to convert pyrolysis oil into commodity chemicals. The analysis constructs a process model for the

system of pyrolysis and bio-oil upgrading, calculates the capital costs of the facility and estimates operating costs to derive an annual return on investment.

Process Model Description

The fast pyrolysis system employs the following steps to convert biomass feedstock to pyrolysis oil: preprocessing, fast pyrolysis, solids removal, pyrolysis oil recovery and heat generation (see Figure 1). During the preprocessing step the biomass is dried to 5% moisture content, chopped, and ground to particles 3mm in diameter. Then the preprocessed biomass is sent to the fast pyrolysis step where the biomass is converted into pyrolysis oil. The pyrolysis reactor consists of a fluidized bed reactor operating at approximate 500^{o}C and ambient pressure in an oxygen-free environment. Table 1 and Table 2 detail the properties of the mixed wood feedstock and the product pyrolysis oil. Compositions of the pyrolysis oils used in each scenario are detailed in the supporting online material of Vispute et al.[10] This information is based on pilot-scale pyrolysis trials at the National Renewable Energy Laboratory (47). These results are particularly relevant to the present analysis as the resulting oil was used in the upgrading investigations of Vispute et al.[10]

The pyrolysis oil contains solid particles such as ash and char, which must be removed before upgrading. In the solids removal step, cyclonic separators with assumed collection efficiency of 90% are employed to remove solids particles from gas/vapor/aerosol stream. The process stream enters the pyrolysis oil recovery stage, which cools the product, recovers vapors and aerosols as pyrolysis oil, and directs non-condensable gases to process heat operations. Although a wide

variety of bio-oil recovery systems have been proposed, this analysis assumes pyrolysis oil is recovered in a single unit operation (quenching with cold liquid). To provide process heat to the biomass drier and the pyrolyzer, a heat generation step is included, which burns the non-condensable gases and a fraction of the char. A small part of the non-condensable gas is recycled as carrier gas for the fluidized bed reactor.

Five scenarios are analyzed for the ICP conversion of the WPO and APPO (see Figure and Table 3). Hydrogen is purchased from external sources, which contributes to relatively high carbon conversion (as opposed to reforming hydrogen from part of the pyrolysis oil). Scenario 1 employs a FCC reactor to catalytically crack the WPO to aromatic hydrocarbons and olefins over a HZSM-5 catalyst at 600°C and atmospheric pressure. In Scenario 2, single-stage hydrotreating of the WPO is first carried out at 125°C and 100 bar pressure over a Ru/C catalyst in a low temperature hydrotreater before the upgraded pyrolysis oil enters the FCC reactor. Hydrotreating converts the WPO to light alkenes which are sent to a FCC reactor for catalytic cracking to aromatic hydrocarbons and olefins. In Scenarios 3, 4, and 5 the WPO is phase-separated into water-insoluble and aqueous phases before being hydrotreated and/or catalytically cracked. This separation is achieved through the liquid-liquid (L-L) extractor shown in Figure 2. The carbohydrate-rich APPO undergoes further processing while the phenol oligomer-rich water insoluble fraction (WIBO) is sold as boiler fuel. The value of WIBO is assumed to be $20/MT, approximately half of the price of coal used for electricity generation in 2010 (48). In more advanced scenarios, the WIBO might be expected to be converted into higher value products like asphalt binders, but these have yet to be commercially developed.[49]

In Scenario 3 the extracted APPO is sent directly to the FCC reactor and passed over a HZSM-5 catalyst at 600°C. In Scenario 4 the APPO first undergoes single-stage hydrotreating at 125°C and 52 bar pressure before being converted via FCC into aromatic hydrocarbons and olefins. In Scenario 5 the APPO undergoes a two-stage hydrotreating process. The first stage occurs at the comparatively low temperature of 125°C and 100 bar pressure over a Ru/C catalyst and the second stage is carried out at 250°C and 100 bar pressure over a Pt/C catalyst. Following the two-stage hydrotreating process the resulting C_1-C_4 alkanes, gasoline cuts, and C_2-C_6 diols are sent to the FCC reactor for production of aromatic hydrocarbons and olefins. Further details on the five scenarios are available in Vispute et al.[10] and Vispute.[50]

Table 4 provides the material flow and consumption rates of the fast pyrolysis facility and Table 5 provides the product yields from the fast pyrolysis of mixed wood feedstock. Table 6 details the cost of the mixed wood feedstock, hydrogen, and Pt, Ru, and zeolite catalysts.

The ICP pathway is modeled using Apsen Plus™ software for the daily conversion of 2000 dry metric tons per day (MTDP) of a mixed wood feedstock into pyrolysis oil, char, and syngas via fast pyrolysis. The fluidized bed reactor is modeled by a RYIELD module in Aspen Plus™ which employs input-output data to simulate the conversion of biomass to pyrolysis oil on a mass balance. The RYIELD model is used to calculate yield distributions. Pyrolysis product yields are from NREL experimental data (47) while hydroprocessing data is from Vispute et al. (10) RYIELD also requires input and output specifications. The input-output data are from the pyrolysis oil analysis based on mixed wood biomass from NREL (47). The FCC process is modeled as five main components: a boiler, a regenerator, a reactor, a distillation column, and a separator. The hydrotreater consists of a reactor packed with a Ru/C or Pt/C catalyst. The

hydrotreaters and FCC reactors are also modeled by a RYIELD module in Aspen Plus™. Carbon selectivity and final product yields presented in Vispute et al.[10] are adopted as the input-output data (see Table 7 for prices and Table 8 for quantities). Due to the availability of different upgrading pathways, different carbon selectivities for olefins and aromatics are obtained for the five scenarios which results in assorted final yields of the biobased commodity chemicals (see Table 9). A higher mass yield of the commodity chemicals may be achieved for higher capital and operating costs.

Equipment costs are estimated with the Aspen Economic Analyzer software. Peters and Timmerhaus factors are employed to estimate the total project cost (see Table 10) (51). A modified version of a discounted cash flow rate of return (DCFROR) spreadsheet developed by NREL is employed to estimate the IRR over a 20 year period.

While commodity chemicals are the facility's principle products, the fast pyrolysis pathway also produces two lower value co-products, char and syngas. Char is capable of being combusted as a coal-substitute in power plants for electricity generation and has value as such.[17] We assume that the char produced by the facility is sold for $20/MT, a value based on the January 2011 price of coal and char's lower relative heating value. This generates an annual income of $1 million for a 2000 MTDP facility. All of the syngas and a fraction of the char produced via fast pyrolysis are combusted within the facility for process heat, reducing the income-generating potential of these co-products.

Results

Installed equipment costs for the five scenarios are summarized in Figure 3. The five scenarios incur similar capital costs for a 2000 metric TPD facility, ranging from a low of $99 million for Scenario 1 to a high of $112 million for Scenario 5. Differences in installed equipment costs are primarily a function of the number of upgrading steps employed: installed equipment costs for upgrading are $20 million for a facility employing only FCC, $24 million for a facility employing a single hydrotreating stage and FCC, and $33 million for a facility employing two hydrotreating stages and FCC (see Figure 3). Other major operations (storage, pretreatment, pyrolysis and oil recovery, and combustion) have roughly the same equipment costs except that additional upgrading adds an additional 5-10% cost to capital expenditures.

The additional capital, catalyst, and hydrogen costs similarly influence operating costs. Scenario 1 incurs annual operating costs of $74.5 million while Scenario 5 incurs annual operating costs of $91 million (see Figure 4). The expense of merchant hydrogen for hydrotreating is responsible for much of this difference, which ranges from zero expenditure for facilities employing only FCC to $16 million annually for those employing two-stage hydrotreating and FCC. This is most evident when comparing hydrogen costs for Scenarios 2 and 4. Both employ single-stage hydrotreating and FCC and 60% more pyrolysis oil is hydrotreated under Scenario 2 than Scenario 4. Scenario 4 consumes 430% more hydrogen per 100g carbon in the feed than Scenario 2,[10] however, and a facility employing Scenario 4 therefore spends $7 million more on hydrogen annually than a facility employing Scenario 2, despite hydrotreating less pyrolysis oil.

Although the additional processing steps incur slightly higher capital and operating costs, the increase in yields of commodity chemicals provides an income stream that more than off-sets

these costs. The 20% increase in installed equipment costs and 22% increase in annual operating costs from Scenario 1 to Scenario 5 results in a 140% increase in the total chemicals yield. Scenario 1, which employs only a FCC stage, produces the lowest quantity of chemicals, while Scenario 5, which employs two hydrotreating stages and a FCC stage, produces the greatest quantity of chemicals. The FCC scenario without hydrotreating has roughly the same effect on the yields of chemicals for WPO and APPO feedstocks (Scenarios 1 and 3). On the other hand, FCC with hydrotreating has a much greater effect on chemical yields from APPO than from WPO (Scenarios 2 and 4). A summary of the chemicals yields in this study are presented in Table 11. The chemicals yields from APPO are higher than those from WPO due to the significantly higher aromatic and olefin carbon yields in the former (approximately 60% more) and higher coke yields in the latter (approximately 100% more) despite the use of identical processing methods in Scenarios 2 and 4. It is likely that this is the result of APPO's lower lignin content.

It should be noted that Vispute et al.[10] in calculating the economic potential of the ICP pathway assumed a pyrolysis oil yield of 70 wt% when in fact the actual yield from the NREL pyrolyzer that produced the pyrolysis oil for their experimental study was only 52 wt% (47). Recognizing that oil yields strongly influence the economic viability of chemical production, we employ the actual 52 wt% yield for the baseline case while also examining pyrolysis oil yields of 60 wt%, 65 wt%, and 70 wt%, which are within the realm of possible yields.

As illustrated in Table 12, FCC scenarios with hydroprocessing, whether using WPO or APPO as feedstock, generate the lowest IRRs. An IRR of <-100% indicates that investors would lose their entire investment within the 20 years covered by the analysis. Scenarios 1 and 3 fall into this

category except for the highest WPO yield for Scenario 1. This is due to low chemical yields when only FCC is employed to upgrade WPO or APPO. Both single and two-stage hydrotreating significantly increase chemicals yields, although IRRs are negative for all but the highest pyrolysis oil yield (70 wt%) for single stage hydrotreating of WPO prior to FCC. Internal rates of return are positive for single and two-stage hydrotreating of APPO prior to FCC, ranging from 1.2% for single stage hydrotreating of pyrolysis oil produced at 52 wt% yield to 14% for two stage hydrotreating of pyrolysis oil produced at 70 wt% yield. These fall short of the 25% IRR usually considered as the threshold for securing capital investment in new processing technology (52).

The results of this analysis are less optimistic about the prospects for commodity chemicals from pyrolysis oil than projected by Vispute et al., who calculated the economic potential of a 100 metric ton per hour (MTPH) mixed wood fast pyrolysis facility employing each of the five ICP scenarios. Using the same assumptions as those used to calculate the economic potential in Vispute et al.,[10] we find much lower average annual net incomes, as illustrated in Table 12. Whereas Vispute et al. roughly estimated annual net incomes ranging between $18 million to $70 million for the five scenarios, our more detailed analysis indicates that annual net incomes will range from negative (-$26.2 million) to no more than $34.2 million.

Sensitivity Analysis

The IRR of a biobased chemicals facility is expected to be sensitive to a number of factors including costs of biomass feedstock, hydrogen, electricity, and labor; income tax rates; and

selling prices of chemical products. Sensitivity analyses were performed on Scenarios 2 (single stage hydrotreating and FCC of the WPO) and 5 (two stage hydrotreating and FCC of the APPO) as shown in Figure 5 and 6, respectively. Both sensitivity analyses assume a 70 wt% pyrolysis oil yield. Internal rate of return is most sensitive to market price of petrochemicals and feedstock costs for both scenarios, although the greatest sensitivity occurs for Scenario 2. A 25% reduction in the market price of petrochemicals under Scenario 2 causes facility IRR to fall from 0.14% to -23.29%. A 25% increase in price causes facility IRR to increase from 0.14% to 8.56%. The same price movements in Scenario 5 result in IRR moving from 14.32% to as low as 4.92% and as high as 22.91%.

Hydrogen cost, labor cost, electricity price, and the income tax rate have very little impact on the facility IRR under Scenario 2. Facility IRR under Scenario 5 is more sensitive to hydrogen cost and the income tax rate due to its use of a two-stage hydrotreating process and the generation of profits on which income tax can be applied. The results of these sensitivity analyses suggest that the economic feasibility of the ICP pathway will be determined by market factors rather than favorable income or payroll tax treatment. Government attempts to improve the profitability of renewable thermochemical processing technologies via income and payroll tax incentives will have a minimal impact relative to changes in the value of processing inputs and outputs. A similar result has been reported for transportation fuel production via fast pyrolysis and upgrading.[53]

An analysis of monthly spot prices of petroleum (average of Brent and WTI crude)[54] and petrochemicals (the total value of BTX, butylene, ethylene, and propylene produced from 1 MT of pyrolysis oil via ICP)[13] from April 1993 to July 2011 shows a strong correlation between the

two (R^2 = 0.8999) (see Figure 7). This correlation has important implications for the IRR of a facility employing fast pyrolysis and ICP to produce commodity chemicals, as the price of petroleum has been very volatile throughout the 21st century. The sensitivity analysis of such a facility's IRR to the price of petrochemicals shows that a 25% increase in the price of petroleum is expected to increase the annual return on investment (ROI) for ICP to within the 25% target for commercializing new technologies (see Figure 6). One metric ton (MT) of raw pyrolysis oil produces $635 of BTX, butylene, ethylene, and propylene at January 2011 petroleum prices when upgraded via ICP (see Tables 7 and 8). A 25% increase in this value represents $791/MT, a level historically reached by petrochemicals prices in June 2008 and May 2011 at 2010 dollars.[13]

The regression analysis presented in Figure 7 allows us to calculate the price of petroleum that correlates with the $791/MT commodity chemicals value to be $927/MT, a sustained price not projected to be reached until 2030.[55] This threshold has been breached in the past, however, most notably during the summer of 2008. Given the high volatility of the petroleum price, it is not unrealistic to expect it to breach this threshold prior to 2030 as well. Furthermore, the continued replacement of petroleum-based fuels with ethanol fuel can be expected to cause the price of petrochemicals to increase beyond what the price of petroleum would suggest.[56]

Further research is needed on ways in which a facility employing fast pyrolysis with ICP can take advantage of this sensitivity to maintain a high IRR despite the volatility of petrochemicals prices. One possible solution is the development of a fast pyrolysis facility capable of alternating between the following two pyrolysis oil upgrading pathways in response to market price shifts: production of transportation fuels (gasoline and diesel) via hydroprocessing, as detailed in

Wright et al.,[57] and production of commodity chemicals via ICP. An analysis of monthly petrochemical and transportation fuel prices since 1993[13, 14, 58] finds that the values of the two upgrading pathways, as defined by the market values of products derived from one MT of pyrolysis oil by each, revolve around one another, changing positions every few years (see Figure 8).

A facility capable of switching between upgrading pathways and subsequent products will be able to ensure that it is always employing the pathway with the greater market value output, regardless of fluctuations in the value of commodity chemicals versus transportation fuels. Whereas the fast pyrolysis pathway is unable to generate sufficient IRRs (>25%) for either transportation fuel production[3] or commodity chemical production based on current market prices, the ability to maximize annual ROI by changing product type in response to changing prices may enhance facility IRR enough to merit capital investment. It is also possible that higher capital and operating costs necessitated by employment of such a capability could outweigh any resulting increases in income.

Conclusion

This paper determines the IRR of a facility producing biobased chemicals via fast pyrolysis and ICP. Five different scenarios are examined: FCC of WPO (Scenario 1); hydrotreating and FCC of WPO (Scenario 2); FCC of APPO (Scenario 3); hydrotreating and FCC of APPO (Scenario 4); and two-stage hydrotreating and FCC of APPO (Scenario 5). Additionally, each scenario is

examined under four different pyrolysis oil yield assumptions: 52 wt%, 60 wt%, 65 wt%, and 70 wt%.

The yields of commodity chemicals derived from each unit of pyrolysis oil are determined by the number of process steps employed by the facility. Output for this 2000 MTPD facility ranged as low as 93.3 MTPD of chemicals for Scenario 1 to as high as 223.8 MTPD of chemicals for Scenario 5. The higher output of commodity chemicals results in more attractive IRRs despite the subsequently greater capital and operating costs, although still not high enough to attract investors at current petrochemicals prices.

Scenarios 1 and 3 generate IRRs of <-100% regardless of pyrolysis oil yield. Indeed, the only two scenarios to generate positive IRRs under the 52 wt% pyrolysis oil yield are those that apply hydrotreating and FCC to the APPO. While facility IRR is as high as 14% when a higher oil yield is assumed (70 wt%), this is still unlikely to be sufficient to merit capital investment (52). Given that the pyrolysis reactor that generated the sample used by Vispute et al.[10] yielded only 52 wt% pyrolysis oil, the most realistic conclusion is that facilities employing the ICP pathway will barely generate a positive IRR. This study demonstrates that, under current market conditions and production technology, such a facility is unlikely to acquire sufficient capital investment to begin operations due to a low potential IRR. This process may become feasible if the commodity chemical prices are favorably high and/or the chemical yields improve significantly.

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Table 1. Properties of mixed wood feedstock

Ultimate Analysis (dry basis)	
Element	**Value (wt %)**
Carbon	47.51
Hydrogen	5.24
Nitrogen	0.28
Chlorine	0.01
Sulfur	0.21
Oxygen	41.05
Proximate Analysis (wet basis)	
Element	**Value (wt %)**
Moisture	5.23
Fixed Content	12.91
Volatile Matter	81.39
Ash	0.48

Source: Czernik S (47)

Table 2. Ultimate analysis of pyrolysis oil

Element	Value (wt %)
Ash	0.06
Water	24.60
Carbon	56.75
Hydrogen	6.17
Nitrogen	0.01
Sulfur	0.03
Oxygen	37.04

Source: Czernik S (47)

1 Table 3. Description of each ICP scenario

Scenario	1	2	3	4	5
Description	WPO is catalytically cracked over HZSM-5 catalyst.	WPO is hydrotreated over Ru/C catalyst and catalytically cracked over HZSM-5 catalyst.	APPO is catalytically cracked over HZSM-5 catalyst.	APPO is hydrotreated over Ru/C catalyst and catalytically cracked over HZSM-5.	APPO is hydrotreated over Ru/C catalyst, hydrotreated over Pt/C catalyst, and catalytically cracked over HZSM-5 catalyst.

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Table 4. Material flow and consumption rate for fast pyrolysis of mixed wood feedstock on a dry basis

Input (dry basis)	Fast Pyrolysis (metric ton/day)
Biomass	2000 [b]
Output (dry basis)	
Char	194 (~150 consumed in combustion)
Pyrolysis oil	1400
Water-soluble fraction[a]	770
Water-insoluble fraction[a]	630
Pyrolysis gas	406 (265 consumed in combustion)

Source: Czernik S (2011, pers. comm.), [a]Vispute[(50)].
[b]Biomass is 25 wt % moisture.

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Table 5. Product yields from fast pyrolysis of mixed wood feedstock

Product Yields	**Fast Pyrolysis (wt%)**
Pyrolysis Gas	36
Pyrolysis Char	12
Pyrolysis Oil	52

Source: Czernik S (2011, pers. comm.)

Table 6. Cost of hydrogen [59, 60] and catalysts [61] used in hydrotreating and FCC

Commodity	**Price ($/kg)**
Hydrogen [a]	3.00
Pt	56.29
Ru	5.60
Zeolite	1.60

[a] Hydrogen's price is calculated as a function of the price of natural gas.

Table 7. Cost of biomass feedstock[3, 62] and prices of commodity chemicals[13, 63]; a * denotes use of benzene price due to unavailability of actual chemical price

Commodity	**Price ($/kg)**
Biomass feedstock	0.08
Aromatics	
Benzene	0.85
Ethyl benzene	1.27
Indene*	0.85
Naphthalene*	0.85
Styrene	1.34
Toluene	0.71
Xylene	0.76
Olefins	
Butylene	0.75
Ethylene	1.49
Propylene	1.58

Table 8. Input-output upgrading process data used for RYIELD specification (Scenario 5; 70 wt% pyrolysis oil yield; pyrolysis oil feed wt%)

Low Temp Hydrotreating Output		High Temp Hydrotreating Output	FCC Output	
Compounds			**Olefins**	
Acetic acid	9.8	5.7	Butylene	5.3
Cyclohexanol	3.3	1.6	Ethylene	12.0
Cyclopentanol	0.3	0.7	Propylene	20.2
Ethanol	0.7	2.0		
Ethylene glycol	24.8	26.3	**Aromatics**	
Glycerol	0	2.7	Benzene	4.0
Hexane	0	3.0	Ethylbenzene	0.4
Levoglucosan	14.8	0	Indene	0.1
Methanol	2.5	3.3	Naphthalene	0.1
Pentane	0	0.4	Styrene	0.2
Propylene glycol	9.6	18.5	Toluene	7.4
Sorbitol	18.9	1.2	Xylene	2.9
Sugars	2.1	0.4		
Tetrahydrofuran	0	0.2	Unidentified	0.4
Tetrahydrofurfuryl	0	2.7	Coke	4.3
γ-Butyrolactone	3.6	4.3	CO	8.4
γ-Valerolactone	0.3	0.5	CO_2	34.4
1,2,3-Butanetriol	0	1.4		
1,2,6-Hexanetriol	0	0.6		
1,2-Butanediol	1.2	5.6		
1,2-Cyclohexanediol	3.3	3.8		
1,2-Hexanediol	0	1.0		
1,4-Butanediol	2.0	2.8		
1,4-Pentanediol	0	0.9		
1-Butanol	0.1	0.4		
1-Pentanol	0	0.3		
1-Propanol	0.3	1.6		
2,3-Butanediol	0	1.4		
2,5-Dimethyl Tetrahydrofuran	0	0.6		
2-Butanol	0	0.5		
2-Hexanol	0	0.2		
2-Methyl Tetrahydrofuran	0	0.7		
3-Methylcyclohexanol	0	1.0		
3-Methylcyclopentanol	0	1.0		
4-Hydroxymethyl-γ-butyrolactone	2.4	1.8		
4-Methylcyclohexanol	0	0.6		

Table 9. Carbon selectivities under different upgrading scenarios [10]

Carbon Selectivity (%)		
Scenario #	**Aromatics**	**Olefins**
1	Benzene: 17.3	Ethylene: 51.8
	Toluene: 40.8	Propylene: 36.6
	Xylene: 23.5	Butylene: 11.6
	EtBenz: 2.0	
2	Benzene: 16.9	Ethylene: 52.2
	Toluene: 37.2	Propylene: 35.9
	Xylene: 38.5	Butylene: 11.4
	EtBenz: 3.4	
3	Benzene: 26.8	Ethylene: 41.6
	Toluene: 46.3	Propylene: 45.9
	Xylene: 20.7	Butylene: 12.4
	EtBenz: 1.2	
4	Benzene: 17.6	Ethylene: 31.8
	Toluene: 45.5	Propylene: 55.4
	Xylene: 31.3	Butylene: 12.8
	EtBenz: 2.6	
5	Benzene: 27.0	Ethylene: 32.0
	Toluene: 49.3	Propylene: 53.8
	Xylene: 19.1	Butylene: 14.2
	EtBenz: 2.3	

1 **Table 10. Methodology for capital cost estimation for nth plant.**

Parameter	Assumption
Total Purchased Equipment Cost (TPEC)	Total 100%
Purchased Equipment	39%
Installation	26%
Instrumentation and Controls	10%
Piping	31%
Electrical Systems	29%
Buildings (including Service Facilities	12%
Total Installed Cost (TIC)	55%
Indirect Cost (IC)	TPEC * Installation Factor (3.02)
Engineering	0.89*TPEC
Construction	32%
Legal and Contractors Fees	34%
Total Direct and Indirect Costs(TDIC)	23%
Contingency	TIC + IC
Fixed Capital Investment (FCI)	20% of TDIC
Working capital (WC)	TDIC + Contingency
Land Use	15% of FCI
Total Capital Investment (with land)	6% of TPEC
	FCI + WC+Land

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1 Table 11. Yield of chemicals vs. yield of pyrolysis oil (kg/hr)

Pyrolysis oil yield	Scenario 1	Scenario 2	Scenario 3	Scenario 4	Scenario 5
52 wt%	4321	6275	4288	9025	10363
60 wt%	5007	7271	4967	10458	12004
65 wt%	5424	7875	5379	11054	13008
70 wt%	5841	8483	5796	12200	14008

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Table 12. 20-year IRR by scenario and pyrolysis oil yield[a]

	IRR by pyrolysis oil yield			
Scenario	**52 wt%**	**60 wt%**	**65 wt%**	**70 wt%**
1	<-100%	<-100%	<-100%	-53.78%
2	-31.17%	-11.12%	-4.30%	0.14%
3	<-100%	<-100%	<-100%	<-100%
4	1.17%	7.03%	8.91%	12.29%
5	4.27%	9.31%	11.92%	14.32%

[a] An IRR of <-100% indicates the facility goes bankrupt in less than 20 years.

Table 12. A comparison of approximate annual net incomes of facilities employing different ICP scenarios ($2/kg H_2, 70 wt% pyrolysis oil yield)

Study	Scenario 1	Scenario 2	Scenario 3	Scenario 4	Scenario 5
Vispute et al.[10]	$18M	$19M	$20M	$50M	$70M
Present analysis	-$26.2M	$9.0M	-$2.8M	$27.6M	$34.2M